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Global trace asymptotics in the self-generated magnetic field in the case of Coulomb-like singularities

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1 Problem

Let us consider the following operator (quantum Hamiltonian) in $\mathbb{R}^d$ with $d=3$

$$H = H_{A,V} = \bigl((hD - A)\cdot \boldsymbol{\sigma}\bigr)^2 - V(x) \tag{1.1}$$

where A, V are real-valued functions and V has a Coulomb-like singularity at 0 or has several such singularities and is smooth and decays as Coulomb or better at infinity[1].

Let $A \in \mathscr{H}^1$. Then operator H is self-adjoint in $\mathscr{L}^2(\mathbb{R}^3, \mathbb{C}^2)$. We are interested in $\operatorname{Tr}^- H_{A,V}$ (the sum of all negative eigenvalues of this operator). Let

$$\mathsf{E}^* = \inf_{A\in \mathscr{H}^1_0(B(0,1))} \mathsf{E}(A), \tag{1.2}$$

$$\mathsf{E}(A) := \Bigl(\operatorname{Tr}^- H_{A,V} + \kappa^{-1}h^{-2}\int |\partial A|^2\, dx\Bigr) \tag{1.3}$$

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[1] In [I5] we assumed that V is a smooth function.

with $\partial A=(\partial_i A_j)$ a matrix.

This paper is the second step to the recovering sharper asymptotics of the ground state energy for atoms and molecules in the self-generated magnetic fields.

Let $\mathsf{x}_j\in\mathbb{R}^3$ ($j=1,\dots,M$, where M is fixed) be singularities ("nuclei"). We assume that

$$V=\sum_{1\le j\le M}\frac{z_j}{\ell_j(x)}+W(x) \tag{1.4}$$

where $\ell_j(x)=\frac{1}{2}|x-\mathsf{x}_j|$,

$$z_j\ge 0,\ \ z_1+\dots+z_M\asymp 1, \tag{1.5}$$

$$|D^\alpha W|\le C_\alpha\sum_{1\le j\le M} z_j\bigl(\ell_j(x)+1\bigr)^{-1}\bigl(\ell_j(x)\bigr)^{-|\alpha|}\qquad\forall\alpha:|\alpha|\le 2 \tag{1.6}$$

but at first stages we will use some weaker assumptions. Later we assume that $V(x)$ decays at infinity sufficiently fast.

In this paper we assume that $\kappa\in(0,\kappa^*]$ where $0<\kappa^*$ is a small constant. As $\kappa=0$ we set $A=0$ and consider $\operatorname{Tr}^- H_{A,V}$; then our results will not be new.

2 Estimates of the minimizer

Let us consider a Hamiltonian with potential V and let A be a minimizing expression (1.3) magnetic field. We say that A is a *minimizer* and in the framework of our problems we will prove it existence.

2.1 Preliminary analysis

First we start from the roughest possible estimate:

Proposition 2.1. *Let $\kappa\le\kappa^*$. Then the near-minimizer A satisfies*

$$|\int\bigl(\operatorname{tr} e_1(x,x,0)-\mathsf{Weyl}_1(x)\bigr)\,dx|\le Ch^{-2} \tag{2.1}$$

and

$$\|\partial A\|\le C\kappa^{\frac{1}{2}} \tag{2.2}$$

Proof. Definitely (2.1)–(2.2) follow from the results of [EFS3] but we give an independent easier proof based on [I5].

(i) First, let us pick up $A = 0$ and consider $\operatorname{Tr}\bigl(\psi_\ell E(0)\psi_\ell\bigr)$ with cut-offs $\psi_\ell(x) = \psi((x - \mathsf{x}_j)/\ell)$ where $\psi \in \mathscr{C}_0^\infty(B(0,1))$ and equals 1 in $B(0,\frac{1}{2})$. Here and below $E(\tau) = \theta(\tau - H_{A,V})$ is a spectral projector of H.

Then

$$|\operatorname{Tr}\bigl(\psi_\ell H^-_{A,V}(0)\psi_\ell\bigr)| \le Ch^{-2} \qquad \text{as} \quad \ell = \ell_* := h^2. \tag{2.3}$$

On the other hand, contribution of $B(x,\ell)$ with $\ell(x) = \frac{1}{2}\min_j |x - \mathsf{x}_j| \ge \ell_*$ to the Weyl error does not exceed $C\rho^2\hbar^{-1} = C\rho^3\ell h^{-1}$ where $\hbar = h/\rho\ell$ in the rescaling; so after summation over $\ell \ge \ell_*$ we get $O(h^{-2})$ provided $\rho^2 \le C\ell^{-1}$. Therefore we arrive to the following rather easy inequality:

$$|\int \bigl(\operatorname{tr} e_1(x,x,0) - \mathsf{Weyl}_1(x)\bigr)\, dx| \le Ch^{-2}. \tag{2.4}$$

This is what rescaling method gives us without careful study of singularity.

(ii) On the other hand, consider $A \ne 0$. Let us prove first that

$$\operatorname{Tr}^-(\psi_\ell H\psi_\ell) \ge Ch^{-2} - Ch^{-2}\int |\partial A|^2\, dx \qquad \text{as} \quad \ell = \ell_*. \tag{2.5}$$

Rescaling $x \mapsto x/\ell$ and $\tau \mapsto \tau/\ell$ and therefore $h \mapsto h\ell^{-\frac{1}{2}} \asymp 1$ and $A \mapsto A\ell^{\frac{1}{2}}$ (because singularity is Coulomb-like), we arrive to the same problem with the same κ (in contrast to section 4 of [I5] where $\kappa \mapsto \kappa\ell$ because of different scale in τ and h) and with $\ell = h = 1$.

However this estimate follows from the proof in section 3 of [ES3] of Lemma 2.1, namely from (3.19)–(3.22) with $Z = d = 1$.

(iii) Consider now ψ_ℓ as in (i) with $\ell \ge \ell_*$. Then according to theorem 4.1 of [I5] rescaled

$$\operatorname{Tr}^-\bigl(\psi_\ell H_{A,V}\psi_\ell\bigr) \ge -C\rho^3\ell h^{-1} - Ch^{-2}\int_{B(x,2\ell/3)} |\partial A|^2\, dx. \tag{2.6}$$

Really, rescaling of the first part is a standard one and in the second part we should have in the front of the integral a coefficient $\kappa^{-1}h^{-2}\rho^2 \times \rho^{-2}\ell(h/\rho\ell)^{-2}$

where factor ρ^2 comes from the scaling of the spectral parameter, factor ρ^{-2} comes from the scaling of the magnitude of A, factor $\ell = \ell^3 \times \ell^{-2}$ comes from the scaling of dx and ∂ respectively, and $h/(\rho\ell)$ is a semiclassical parameter after rescaling. So, we acquire a factor $\rho^2\ell \le C$.

Then

$$\int \bigl(\operatorname{tr} e_1(x,x,0) - \mathsf{Weyl}_1(x)\bigr)\, dx \ge -Ch^{-2} - Ch^{-2}\int |\partial A|^2\, dx \tag{2.7}$$

and adding magnetic field energy we find out that the left-hand expression of (2.1) is greater than the same expression with $A=0$ plus $(C-\kappa^{-1})h^{-2}\|\partial A\|^2$ minus Ch^{-2} which implies (2.1) and (2.2) as A is supposed to be a near-minimizer. $\square$

Remark 2.2. We are a bit ambivalent about convergence of $\int \mathsf{Weyl}_1(x)\, dx$ at infinity, as for Coulomb potential it diverges. In this case however we can either replace $H_{A,V}$ by $H_{A,V}+\eta$ with a small parameter $\eta>0$ or consider the left-hand expression of (2.1) plus magnetic field energy as an object to minimize.

2.2 Rough estimate to a minimizer. I

Let us repeat arguments of subsection 1.3 of [I5]. Let us consider equation for an minimizer A as in (1.13) of [I5]:

$$\Delta A = -2\kappa h^2 \sum_k \bigl(\sigma_j\sigma_k(hD_k - A_k)_x + \sigma_k\sigma_j(hD_k - A_k)_y\bigr) e(x,y,\tau)|_{y=x} \tag{2.8}$$

If we scale with the scale $x\mapsto x/\ell$, $\tau\mapsto\tau/\rho^2$, $h\mapsto \hbar = h/(\rho\ell)$ then (2.8) would become

$$\Delta A = - 2\kappa\rho^3\ell\hbar^2 \sum_k \bigl(\sigma_j\sigma_k(\hbar D_k - \rho^{-1}A_k)_x + \sigma_k\sigma_j(\hbar D_k - \rho^{-1}A_k)_y\bigr) e(x,y,\tau)|_{y=x} \tag{2.9}$$

and since so far $\rho^2\ell = 1$ we arrive to

$$\Delta A = - 2\kappa\rho\hbar^2 \sum_k \bigl(\sigma_j\sigma_k(\hbar D_k - \rho^{-1}A_k)_x + \sigma_k\sigma_j(\hbar D_k - \rho^{-1}A_k)_y\bigr) e(x,y,\tau)|_{y=x}. \tag{2.10}$$

(i) Plugging for $u=E(0)f$ and repeating arguments of [I5] we conclude that in the rescaled coordinates

$$\begin{aligned}(2.11)\quad \|\hbar D_x u\| \le \|((\hbar D_x-\rho^{-1}A_x)\cdot\boldsymbol{\sigma})u\| + C\rho^{-1}\|A\|_6\|u\|_3 \le\\ \|((\hbar D_x-\rho^{-1}A_x)\cdot\boldsymbol{\sigma})u\| + C\rho^{-1}\hbar^{-\frac{1}{4}}\|A\|_6\|u\|^{\frac{3}{4}}\cdot\|\hbar D_x u\|^{\frac{1}{4}}\le\\ \|((\hbar D_x-\rho^{-1}A_x)\cdot\boldsymbol{\sigma})u\| + \frac{1}{2}\|\hbar D_x u\| + C(\rho^{-1}\hbar^{-\frac{1}{4}}\|A\|'_6)^{\frac{4}{3}}\|u\|\end{aligned}$$

where $\|A\|_6$ calculated in the rescaled coordinates is $\ell^{-3/6}\|A\|_{6,\mathsf{orig}}$ (where subscript "orig"means that the norm is calculated in the original coordinates) which does not exceed $C\ell^{-\frac{1}{2}}\|\partial A\|_{\mathsf{orig}}\le C\ell^{-\frac{1}{2}}\kappa^{\frac{1}{2}}$ due to (2.2) and therefore

$$\|\hbar D_x u\| \le C\bigl(1+\rho^{-\frac{3}{4}}h^{-\frac{1}{4}}\ell^{-\frac{1}{4}}\kappa^{\frac{1}{2}}\bigr)^{\frac{4}{3}}\|f\|. \tag{2.12}$$

Continuing arguments of section 1.3 of[I5] we conclude that in the rescaled coordinates

$$\begin{aligned}(2.13)\quad \hbar\|\Delta\partial A\|_{\infty,B(x,1)} + \|\Delta A\|_{\infty,B(x,1)} \le K\ell^{-\frac{1}{2}}\\ K:=C\kappa\hbar^{-1}\bigl(1+\rho^{-1}\hbar^{-\frac{1}{4}}\ell^{-\frac{1}{2}}\kappa^{\frac{1}{2}}\bigr)^4.\end{aligned}$$

Then <u>either</u>

$$\|\partial A\|_{\infty,B(x,\frac{3}{4})} + \|\partial A\|^*_{\infty,B(x,\frac{3}{4})} \le CK\ell^{-\frac{1}{2}} \tag{2.14}$$

<u>or</u>

$$\|\partial A\|_{\infty,B(x,\frac{3}{4})} + \|\partial A\|^*_{\infty,B(x,\frac{3}{4})} \le C\|\partial A\| = C\|\partial A\|_{\mathsf{orig}}\ell^{-\frac{1}{2}} \le C\kappa^{\frac{1}{2}}\ell^{-\frac{1}{2}}. \tag{2.15}$$

where in the rescaled coordinates

$$\|B\|^* := \sup_{x,y}|B(x)-B(y)|\cdot|x-y|^{-1}(1+|\log|x-y||)^{-1}. \tag{2.16}$$

In the latter case (2.15) we have in the original coordinates

$$\|\partial A\|_{\infty,B(x,\frac{3}{4}\ell)} \le C\kappa^{\frac{1}{2}}\ell^{-\frac{3}{2}} \tag{2.17}$$

and we are rather happy because then the effective intensity of the magnetic field in $B(x,\ell)$ is $\rho^{-1}\ell\|\partial A\|_{\infty,B(x,\ell)}\le C\kappa^{\frac{1}{2}}$ if we take $\rho=\ell^{-\frac{1}{2}}$.

In the former case (2.14) let us consider (still in the rescaled coordinates) $\beta(x)=|\partial A(x)|\ell^{\frac{1}{2}}$. Then $\beta(x)$ has the same magnitude $\beta(y)$ in γ-vicinity of y with $\gamma=\epsilon\beta(y)K^{-1}|\log(\beta(y)K^{-1})|^{-1}$ (or $\gamma_1=\epsilon$, whatever is smaller). But then in the rescaled coordinates

$$\ell^{-1}\beta^2(\beta K^{-1}|\log(\beta K^{-1})|^{-1})^3\le C\|\partial A\|^2\le C\|\partial A\|^2_{\mathsf{orig}}\ell^{-1}\le C\kappa^{\frac{1}{2}}\ell^{-1}$$

and then

$$\beta\le C\kappa^{\frac{1}{10}}K^{\frac{3}{5}}|\log(\beta K^{-1})|^{\frac{3}{5}}$$

which implies

$$\beta\le C\hbar^{-\frac{6}{5}}|\log\hbar|^{\frac{3}{5}},\qquad \hbar=h\ell^{-\frac{1}{2}} \tag{2.18}$$

(as $\gamma\asymp 1$ the same arguments lead us to (2.17)).

Therefore in the first round of our estimates we arrive to the estimates in the rescaled coordinates

$$|\partial A|\le\beta\ell^{-\frac{1}{2}},\qquad \beta:=C\hbar^{-\frac{6}{5}-\delta} \tag{2.19}$$

where we just estimated $|\log\hbar|$ by $\hbar^{-\delta_1}$; below we increase δ if needed but it still remains an arbitrarily small exponent.

(ii) In the second round we do not invoke $\|A\|_6$ but rather $\|A\|_{\infty,B(y,\gamma)}\le C\beta\ell^{-\frac{1}{2}}\gamma$ where we consider a ball of radius $\gamma\le 1$ in the rescaled coordinates (and subtract a constant from A if needed), resulting in

$$\|\Delta A\|_{\infty,B(x,\gamma)}\le C\kappa\hbar^{-1}\rho\bigl(1+\beta\gamma\ell^{-\frac{1}{2}}\rho^{-1}\bigr)^4.$$

Let us increase ρ to $\rho'=\bigl(\beta h\ell^{-\frac{3}{2}}\bigr)^{\frac{1}{2}}=C\ell^{-\frac{1}{2}}(\beta\hbar)^{\frac{1}{2}}=C\ell^{-\frac{1}{2}}\hbar^{-\frac{1}{10}-\delta}\ge\ell^{-\frac{1}{2}}$ and use $\gamma=h/\rho'\ell=\hbar^{\frac{11}{10}-\delta}\le 1$. Then we arrive to

$$\|\Delta A\|_{\infty,B(x,\gamma)}\le K\ell^{-\frac{1}{2}},\qquad K:=C\kappa\hbar^{-\frac{7}{5}-\delta}. \tag{2.20}$$

Repeating arguments of the first rounds we conclude that <u>either</u> (2.17) holds <u>or</u>

$$|\partial A|\le\beta\ell^{-\frac{1}{2}},\qquad \beta:=K^{\frac{3}{5}-\delta}\le C\hbar^{-\frac{21}{25}-\delta}; \tag{2.21}$$

then rescaled magnetic field is $O(\beta\ell^{-\frac{1}{2}}/\rho)=O(\hbar^{-21/25-\delta})$. Here we returned to the natural scale (ℓ,ρ) with $\rho=\ell^{-\frac{1}{2}}$.

(iii) One can also run third etc rounds, using partially arguments of subsection 2.1 of [I5]; then the rescaled magnetic field is $O(\hbar^{-\delta})$. However to prove that the rescaled magnetic field $O(1)$ we need to modify them, and we do it in the next subsection.

2.3 Rough estimate. II

In this step we repeat arguments of subsection 2.1 of [I5] but we have a problem: we cannot use $\mu = \|\partial A\|_\infty$ as we have domains $\mathcal{X}_r = \{x : \ell(x) \geq r\}$ rather than the whole space. So we get the following analogue of (2.19) of [I5] in the rescaled coordinates:

$$\|\Delta A\|_{\infty, B(x,\frac{3}{4})} + \hbar \|\Delta \partial A\|_{\infty,\frac{3}{4}} \leq C\kappa\rho\Bigl(\bar{\mu} + \bar{\mu}^{-1}\hbar^{\frac{1}{2}(\theta-1)}\rho^{-\frac{1}{2}}\|\partial A\|^{\frac{1}{2}}_{\mathscr{C}^\theta(B(x,1))}\Bigr) \tag{2.22}$$

with $\bar{\mu} = \max(\mu, 1)$, and $\mu = \rho^{-1}|\partial A|_{\infty, B(x,1)}$. But then

$$\hbar^{\theta-1}\rho^{-1}\|\partial A\|_{\mathscr{C}^\theta(B,(x,\frac{1}{2}))} \leq \epsilon\hbar^{(\theta-1)}\rho^{-1}\|\partial A\|_{\mathscr{C}^\theta(B(x,1))} + C\kappa\mu + C\kappa. \tag{2.23}$$

Obviously in the right-hand expression we can replace $\mu = \rho^{-1}|\partial A|_{\infty, B(x,1)}$ by any other norm, in particular by $\mathscr{L}^2$-norm

$$\mu = \rho^{-1}\|\partial A\|_{B(x,1)} = \rho^{-1}\ell^{-\frac{1}{2}}\|\partial A\|_{\mathsf{orig}}$$

which would be less than $C\kappa^{\frac{1}{2}}$.

Let $\nu(r) = \sup_{x:\,\ell(x)\geq r} f(x)$ where $f(x)$ is the left-hand expression of (2.12) calculated for given x in the rescaled coordinates. Then (2.23) implies that

$$\nu(r) \leq \frac{1}{2}\nu(\frac{1}{2}r) + C\kappa^{\frac{1}{2}}$$

which in turn implies that

$$\nu(r) \leq \frac{1}{2}\nu(2^{-n}r) + 2C, \qquad n \geq 1,$$

and therefore

$$\nu(r) \leq 4C\kappa^{\frac{1}{2}} + 4\sup_{C_0h^2 \leq \ell(x) \leq 2C_0h^2} f(x) \leq C_1\kappa^{\frac{1}{2}}$$

due to the rough estimate (because $\hbar \asymp 1$ as $\ell(x) \asymp h^2$). Then going to the original coordinates we arrive to estimates below:

Proposition 2.3. *Let $\kappa \leq \kappa^*$, $\rho = c\ell^{-\frac{1}{2}}$. Let A be a minimizer. Then for $\ell(x) \geq \ell_* = h^2$ (2.17) holds and also*

$$|\partial^2 A(x) - \partial^2 A(y)| \leq C\kappa^{\frac{1}{2}}\ell^{-\frac{5}{2}}|x-y|^\theta\ell^{\theta/2}\ell_*^{-\theta/2} \qquad 0 < \theta < 1, \tag{2.24}$$

and

$$|\partial A(x) - \partial A(y)| \leq C\kappa^{\frac{1}{2}}\ell^{-\frac{5}{2}}|x-y|(1 + |\log|x-y||). \tag{2.25}$$

Remark 2.4. (i) So far we used only assumption that

$$|\partial^\alpha V| \le C\rho^2 \ell^{-|\alpha|} \qquad \forall \alpha : |\alpha| \le 2 \tag{2.26}$$

with $\rho = \ell^{-\frac{1}{2}}$ but even this was excessive.

(ii) In this framework however we cannot prove better estimates as (2.17) always remains a valid alternative even if $\rho \ll \ell^{-\frac{1}{2}}$.

(iii) Originally we need an assumption (2.4) of [I5] $|V| \ge \epsilon_0$, but for $d \ge 3$ one can easily get rid off it by rescaling technique; see also corollary 2.3(ii).

Consider now zone $\{x : \ \ell(x) \le \ell_*\}$.

Proposition 2.5. *Let $\kappa \le \kappa^*$, $\rho \le c\ell^{-\frac{1}{2}}$. Let A be a minimizer. Then $|\partial A| \le Ch^{-3}$ as $\ell(x) \le \ell_*$.*

Proof. Proof is standard, based on rescaling (then $\hbar = 1$) and equation (2.8) for A. We leave details to the reader. □

Let us slightly improve estimate to A. We already know that $|\partial A(x)| \le C_0\beta$ with $\beta = \ell^{-\frac{3}{2}}$ and using a standard rescaling technique we conclude that

$$|\Delta A| \le C\kappa\rho^2\beta + C\kappa\rho^3\ell^{-1} \tag{2.27}$$

which does not exceed $C\kappa\ell^{-\frac{5}{2}}$ which implies

Proposition 2.6. *In our framework*

(i) As $\ell(x) \ge h^2$

$$|A| \le C\kappa\ell^{-\frac{1}{2}}, \qquad |\partial A| \le C\kappa\ell^{-\frac{3}{2}}, \tag{2.28}$$

$$|\partial A(x) - \partial A(y)| \le C_\theta \kappa \ell^{-\frac{3}{2}-\theta}|x-y|^\theta \qquad \text{as } |x-y| \le \frac{1}{2}\ell(x) \tag{2.29}$$

for any $\theta \in (0,1)$

(ii) as $\ell(x) \le h^2$ these estimates hold with $\ell(x)$ replaced by h^2.

Here in comparison with old estimates we replaced factor $\kappa^{\frac{1}{2}}$ by κ which is an advantage.

Consider now zone $\{\ell \ge \max(a,1)\}$ and assume that

$$\rho \le C\ell^{-\nu} \qquad \text{as}\quad \ell \ge \frac{1}{2} \tag{2.30}$$

with $\nu > 1$. Then if also $\beta = O(\ell^{-\nu_1})$ as $\ell \ge 1$ the right hand expression of (2.27) does not exceed $C\kappa(\ell^{-3\nu-1} + \ell^{-\nu_1-2\nu})$ and therefore we almost upgrade estimate to β to $O(\ell^{-3\nu} + \ell^{-\nu_1-2\nu+1})$ and repeating these arguments sufficiently many times to $O(\ell^{-3\nu})$. However, there are obstacles: first, as $\nu > 1$ we get

$$A_j = \sum_m \alpha_{j,m}|x - x_m|^{-1} + O(\ell^{-1-\delta})$$

with constant $\alpha_{j,m}$; however assumption $\nabla\cdot A = 0$ implies $\alpha_{j,m} = 0$ and we pass this obstacle. The second obstacle

$$A_j = \sum_{k,m} \alpha_{jk,m}(x_k - x_{k,m})|x - x_m|^{-3} + O(\ell^{-2})$$

with constant $\alpha_{jk,m}$ we cannot pass as assumption $\nabla\cdot A = 0$ implies only that modulo gradient $A = \sum_m \beta_m \times \nabla \ell_m^{-1}$ with constant vectors β_m and one cannot pass this obstacle.

Therefore we upgrade (2.28)–(2.29) there:

Proposition 2.7. *In our framework assume additionally that* (2.30) *holds. Then as* $\nu > \frac{4}{3}$

$$|A| \le C\kappa\ell^{-2}, \qquad |\partial A| \le C\kappa\ell^{-3}, \tag{2.31}$$

$$|\partial A(x) - \partial A(y)| \le C_\theta \kappa \ell^{-3-\theta}|x-y|^\theta \qquad \text{as}\quad |x-y| \le \frac{1}{2}\ell(x) \tag{2.32}$$

as $\ell(x) \ge 1$ *(for all* $\theta \in (0,1)$*).*

Remark 2.8. (i) In application we are interested in $\nu = 2$;

(ii) We cannot improve (2.31)–(2.32) no matter how fast ρ decays.

3 Tauberian theory

Recall that the standard Tauberian theory results in the remainder estimate $O(h^{-2})$. Really, as the rescaled magnetic field intensity is no more than

$C\kappa^{\frac{1}{2}}$, contribution of $B(x,\ell(x))$ to the Tauberian error does not exceed $C\rho^2\times\hbar^{-1} = C\rho^3\ell h^{-1}$ which as $\rho\asymp\ell^{-\frac{1}{2}}$ translates into $C\ell^{-\frac{1}{2}}h^{-1}$ and summation over $\{x: \ell(x)\ge\ell_*=h^2\}$ results in Ch^{-2}. On the other hand, contribution of $\{x:\ell(x)\le\ell_*=h^2\}$ into asymptotics does not exceed $C\hbar^{-3}\ell_*^{-1}=Ch^{-2}$ as $\hbar=1$.

However now we can unleash arguments of [IS]. Recall that we are looking at

$$\mathsf{Tr}(\psi H^-_{A,V}\psi)=\mathsf{Tr}(\phi_1 H^-_{A,V}\phi_1)+\mathsf{Tr}(\phi_2 H^-_{A,V}\phi_2) \tag{3.1}$$

where $\psi^2=\phi_1^2+\phi_2^2$, $\operatorname{supp}\phi_1\subset\{x,|x|\le 2R\}$, $\operatorname{supp}\phi_2\subset\{x,R\le|x|\le a\}$ and we compare it with the same expression calculated for H_{A,V^0} with $V^0=z|x|^{-1}$. Here we assume that

$$a\le 1,\qquad z\asymp 1 \tag{3.2}$$

and

$$|D^\alpha(V-V^0)|\le c_0a^{-1}\ell^{-|\alpha|}\qquad\forall\alpha:|\alpha|\le 3. \tag{3.3}$$

The latter assumption is too restrictive and could be weaken. Then

$$\mathsf{Tr}\bigl(\phi_2(H^-_{A,V}-H^-_{A,V^0})\phi_2\bigr)=\\ \int\bigl(\mathsf{Weyl}_1(x)-\mathsf{Weyl}_1^0(x)\bigr)\,\phi_2^2(x)\,dx+O(R^{-\frac{1}{2}}h^{-1}) \tag{3.4}$$

where Weyl_1^0 and Weyl^0 are calculated for operator with potential V^0. Really, we prove this for each operator $H_{A,V}$ and H_{A,V^0} separately[2].

On the other hand, considering $V^\zeta=V^0(1-\zeta)+V\zeta=V^0+W\zeta$ and following [IS] we can rewrite the similar expression albeit for $\phi_2=1$ as

$$\mathsf{Tr}\int_0^1 W\theta(-H_{A,V^\zeta})\,d\zeta \tag{3.5}$$

and applying the semiclassical approximation (under temporary assumption that W is supported in $\{x:\ |x|\le 4R\}$) one can prove that as $\phi_1=1$

$$\mathsf{Tr}\bigl(\phi_1(H^-_{A,V}-H^-_{A,V^0})\phi_1\bigr)=\\ \int\bigl(\mathsf{Weyl}_1(x)-\mathsf{Weyl}_1^0(x)\bigr)\,\phi_1^2(x)\,dx+O(a^{-1}Rh^{-2}). \tag{3.6}$$

[2] Sure, such formula requires two-term expression but one can verify easily that the second term is 0.

Really, contribution of ball $B(x,\ell(x))$ does not exceed $Ca^{-1}\hbar^{-2}=Ca^{-1}\ell(x)h^{-2}$ and summation with respect to partition as $\ell(x)\le R$ returns $Ca^{-1}Rh^{-2})$; meanwhile contribution of $\{x:\ell(x)\le \ell_*\}$ does not exceed $Ca^{-1}\hbar^{-2}=Ca^{-1}$ as there $\hbar=1$.

One can get rid off the temporary assumption and take ϕ_1 supported in $\{x:\ell(x)\le 2R\}$ instead.

Therefore we arrive to

Proposition 3.1. *Under assumption* (3.3)

$$\operatorname{Tr}\bigl(\psi(H^-_{A,V}-H^-_{A,V^0})\psi\bigr)=\\
\int \bigl(\mathsf{Weyl}_1(x)-\mathsf{Weyl}_1^0(x)\bigr)\,\psi^2(x)\,dx+O\bigl(a^{-\frac{1}{3}}h^{-\frac{4}{3}}\bigr) \tag{3.7}$$

Really, $a^{-\frac{1}{3}}h^{-\frac{4}{3}}$ is $R^{-\frac{1}{2}}h^{-1}+a^{-1}Rh^{-2}$ optimized by $R\asymp R_*:=(ah)^{\frac{2}{3}}$; as $h^2\le a$ we note that $h^2\le R_*\le a$.

Corollary 3.2. *(i) As $M=1$ equality* (3.7) *remains valid with $\psi=1$ and $a=1$.*

(ii) As $M\ge 2$ and $a\ge h^2$ equality (3.7) *becomes*

$$\operatorname{Tr}\bigl(\psi(H^-_{A,V}-H^-_{A,V^0})\psi\bigr)=\\
\int \bigl(\mathsf{Weyl}_1(x)-\mathsf{Weyl}_1^0(x)\bigr)\,\psi^2(x)\,dx+O\bigl((a^{-\frac{1}{3}}+1)h^{-\frac{4}{3}}\bigr) \tag{3.8}$$

where we reset case $a\ge 1$ to $a=1$.

Remark 3.3. One can apply much more advanced arguments of [I3] or section 12.5 of [I4]. Unfortunately using these arguments so far I was not able to improve the above results unless $\kappa\ll 1$. More precisely, I proved estimate $O(\kappa h^{-\delta-\frac{4}{3}}+h^{-1})$ as $a=1$ (or even $o(h^{-1})$ as $a\gg 1$, $\kappa=o(h^{\frac{1}{3}+\delta})$ and some assumptions of global nature are fulfilled). However as I still hope to improve these results, I am not including them here.

4 Single singularity

4.1 Coulomb potential

Consider now exactly Coulomb potential: $V = z|x|^{-1}$. Then according to Theorem 2.4 of [EFS3] as $h = 1$, $z = 1$ and $0 < \kappa \le \kappa^*$

$$\lim_{R\to\infty}\Bigl(\inf_A\Bigl(\operatorname{Tr}^-(\phi_R H_A\phi_R) + \frac{1}{\kappa}\int |\partial A|^2\,dx\Bigr) - \int \mathsf{Weyl}_1(x)\phi_R^2(x)\,dx\Bigr) =: 2z^2 S(z\kappa). \tag{4.1}$$

which according to Lemma 2.5 of [EFS3] coincides with

$$\lim_{\eta\to 0^+}\Bigl(\inf_A\Bigl(\operatorname{Tr}^-(H_A+\eta) + \frac{1}{\kappa}\int |\partial A|^2\,dx\Bigr) - \int \mathsf{Weyl}_1(H_A+\eta, x)\,dx\Bigr) = 2z^2 S(z\kappa). \tag{4.2}$$

Here $\phi \in \mathscr{C}_0^\infty(B(0,1))$, $\phi = 1$ in $B(0,\frac{1}{2})$, $\phi_R = \phi(x/R)$. Also due to scaling for $z > 0$ one has a Scott coefficient $2z^2 S(\kappa z)$.

Proposition 4.1. *As* $0 < \kappa < \kappa'$

$$S(\kappa') \le S(\kappa) \le S(\kappa') + C\kappa'(\kappa^{-1} - \kappa'^{-1}). \tag{4.3}$$

Proof. Monotonicity of $S(\kappa)$ is obvious.

Let $0 < \kappa < \kappa' < \kappa'' \le \kappa^*$. Then for any $\varepsilon > 0$ if $R = R_\varepsilon$ is large enough then the left-hand expression in (4.1) for κ' (without $\inf$ and $\lim$) is greater than $S(\kappa'') - \varepsilon + (\kappa'^{-1} - \kappa''^{-1})\|\partial A\|^2$; also, if A is an almost minimizer there, it is less than $S(\kappa') + \varepsilon$.

Therefore $(\kappa'^{-1} - \kappa''^{-1})\|\partial A\|^2 \le |S(\kappa'') - S(\kappa')| + 2\varepsilon$. But then

$$\begin{aligned} S(\kappa) - \varepsilon \le S(\kappa') + \varepsilon + (\kappa^{-1} - \kappa'^{-1})\|\partial A\|^2 \le \\ S(\kappa') + \varepsilon + C(\kappa^{-1} - \kappa'^{-1})(\kappa'^{-1} - \kappa''^{-1})^{-1}\bigl(|S(\kappa'') - S(\kappa')| + 2\varepsilon\bigr) \end{aligned}$$

and therefore

$$(\kappa^{-1} - \kappa'^{-1})^{-1}|S(\kappa) - S(\kappa')| \le (\kappa'^{-1} - \kappa''^{-1})^{-1}|S(\kappa') - S(\kappa'')| \tag{4.4}$$

which for $\kappa'' = \kappa^*$ implies (4.3). $\square$

Remark 4.2. Using global equation (2.8) we conclude that as

$$|\partial^\alpha A| \le C\kappa \ell^{-1-|\alpha|} \qquad \ell \ge 1,\ |\alpha|\le 1, \tag{4.5}$$

$$|\partial^\alpha A| \le C\kappa \ell^{-\frac{1}{2}-|\alpha|} \qquad \ell \le 1,\ |\alpha|\le 1, \tag{4.6}$$

$$\|\partial A\|^2 \le C\kappa^2. \tag{4.7}$$

Then

$$S'(\kappa) \le C, \qquad |S(\kappa(1+\eta)) - S(\eta)| \le C\kappa\eta. \tag{4.8}$$

4.2 Main theorem

In the "atomic" case $M=1$ we arrive instantly to

Theorem 4.3. *If $M=1$, $\kappa\le\kappa^*$ then*

$$\mathsf{E}^* = \int \mathsf{Weyl}_1(x)\,dx + 2z^2 S(z\kappa)h^{-2} + O(h^{-\frac{4}{3}}). \tag{4.9}$$

Proof. If A satisfies minimizer properties then in virtue of corollary 3.2

$$\mathsf{Tr}^- H_{A,V} - \int \mathsf{Weyl}_1(x)\,dx \equiv \mathsf{Tr}^- H_{A,V^0} - \int \mathsf{Weyl}_1^0(x)\,dx \mod O(h^{-\frac{4}{3}}) \tag{4.10}$$

and adding magnetic energy and plugging either minimizer for V or for V^0 we get

$$\begin{aligned}\inf_A\Bigl(\mathsf{Tr}^- H_{A,V} - \int \mathsf{Weyl}_1(x)\,dx + \frac{1}{\kappa h^2}\int |\partial A|^2\,dx\Bigr) \lesseqgtr \\ \inf_A\Bigl(\mathsf{Tr}^- H_{A,V^0} - \int \mathsf{Weyl}_1^0(x)\,dx + \frac{1}{\kappa h^2}\int |\partial A|^2\,dx\Bigr) \pm Ch^{-\frac{4}{3}}.\end{aligned} \tag{4.11}$$

Sure as V (and surely V^0) are not sufficiently fast decaying at infinity the left (and for sure the right hand) expression in (4.10) should be regularized as in section 4. However for potential decaying fast enough (faster than $|x|^{-2-\delta}$) regularization is not needed.

For V^0 we have an exact expression which concludes the proof. □

5 Several singularities

Consider now "molecular" case $M \geq 1$. Then we need more delicate arguments.

5.1 Decoupling of singularities

Consider partition of unity $1 = \sum_{0\le j\le m} \psi_j^2$ where ψ_j is supported in $\frac{1}{3}a$-vicinity of x_j as $j = 1, \dots, m$ and $\psi_0 = 0$ in $\frac{1}{4}a$-vicinities of x_j ("near-nuclei" and "between-nuclei" partition elements).

Estimate from above

Then

$$\operatorname{Tr} H^-_{A,V} = \sum_{0\le j\le m} \operatorname{Tr}(\psi_j H^-_{A,V}\psi_j) \tag{5.1}$$

and to estimate E^* from the above we impose an extra condition to A:

$$A = 0 \qquad \text{as} \quad \ell(x) \geq \frac{1}{5}a. \tag{5.2}$$

Then in this framework we estimate

$$|\operatorname{Tr}^-(\psi_0 H^-_{A,V}\psi_0) - \int \mathsf{Weyl}_1(x)\psi_0^2(x)\,dx| \leq Ch^{-1}a^{-\frac{1}{2}}. \tag{5.3}$$

Proof is trivial by using ℓ-admissible partition and applying results of the theory without any magnetic field.

So, to estimate E^* from above[3] we just need to estimate from above minimum with respect to A satisfying (5.2) of expression

$$\operatorname{Tr}(\psi_j H^-_{A,V}\psi_j) - \int \mathsf{Weyl}_1(x)\psi_j^2(x)\,dx + \frac{1}{\kappa h^2}\int_{\{\ell_j(x)\le \frac{1}{5}a\}} |\partial A|^2\,dx. \tag{5.4}$$

[3] Modulo error in (3.8).

Estimate from below

In this case we use the same partition of unity $\{\psi_j^2\}_{j=0,1,\dots,m}$ and estimate

$$\operatorname{Tr} H^-_{A,V} \ge \sum_{0\le j\le m} \operatorname{Tr}^-(\psi_j H_{A,V'}\psi_j) \tag{5.5}$$

with

$$V' = V + 2h^2\sum_j (\partial\psi)^2 \tag{5.6}$$

and we also use decomposition

$$\int |\partial A|^2\,dx = \sum_{0\le j\le m}\int \omega_j^2|\partial A|^2\,dx \tag{5.7}$$

with

$$\omega_j(x)=1 \quad\text{as}\quad \ell_j(x)\le \frac{1}{10}a,\qquad \omega_j(x)\ge 1-C\varsigma\quad\text{as}\quad \ell_j(x)\le\frac{1}{2}a \\ j=1,\dots,m, \tag{5.8}$$

$$\omega_0\ge\epsilon_0\varsigma\quad\text{as}\quad \ell(x)\ge\frac{1}{5}a. \tag{5.9}$$

So far $\varsigma>0$ is a constant but later it will be a small parameter. Then since

$$\operatorname{Tr}^-(\psi_0 H_{A,V'}\psi_0) - \int \mathsf{Weyl}_1(x)\psi_0^2(x)\,dx + \frac{1}{\kappa h^2}\int \omega_0^2|\partial A|^2\,dx \ge \\ Ch^{-1}a^{-\frac{1}{2}} \tag{5.10}$$

(again proven by partition) in virtue of [I5] we are left with the estimates from below for

$$\operatorname{Tr}^-(\psi_j H_{A,V'}\psi_j) - \int \mathsf{Weyl}_1(x)\psi_j^2(x)\,dx + \frac{1}{\kappa h^2}\int \omega_j^2|\partial A|^2\,dx. \tag{5.11}$$

Remark 5.1. (i) Note that the error in Weyl_1 when we replace V' there by V does not exceed $Ch^{-1}(1+a^{-\frac{1}{2}})$ which is less than error in (3.8). Here we can also assume that A satisfies (5.2); we need just to replace ς by $\epsilon_0\varsigma$ in (5.8)–(5.9).

(ii) We also can further go down by replacing $\operatorname{Tr}^-(\psi_j H_{A,V'}\psi_j)$ by $\operatorname{Tr}(\psi_j H^-_{A,V'}\psi_j)$.

(iii) Therefore we basically have the same object for both estimates albeit with marginally different potentials (V in the estimate from above and V' in the estimate from below) and with a weight ω_j^2 satisfying (5.8)–(5.9); in both cases $\omega = 1$ as $\ell(x) \le \frac{1}{10}a$ but in the estimate from above $\omega(x)$ grows to C_0 and in the estimate from below $\omega(x)$ decays to ς as $\ell(x) \ge \frac{1}{3}a$ and in both cases condition (5.2) could be imposed or skipped.

(iv) From now on we consider a single singularity at 0 and we skip index j. However if there was a single singularity from the beginning, all arguments of this and forthcoming subsections would be unnecessary.

Scaling

(i) We are done as $z \asymp 1$ but as $z \ll 1$ [4] we need a bit more fixing. The problem is that $V \asymp z\ell^{-1}$ only as $|x| \le za$; otherwise $V \lesssim a^{-1}$ (where we assume that $a \le 1$). To deal with this we apply in the zone $\{x :\ za \le |x| \le a\}$ the same procedure as before and its contribution to the error will be $Ch^{-1}a^{-\frac{1}{2}}$ as $\rho = a^{-\frac{1}{2}}$ here. Actually we also need to keep $|x| \ge z^{-1}h^2$; so we assume that $z^{-1}h^2 \le za$ i.e. $z \ge a^{-\frac{1}{2}}h$.

Now scaling $x \mapsto x' = x/za$, multiplying $H_{a,V}$ by a (and therefore also multiplying A by $a^{\frac{1}{2}}$, so $A \mapsto A' = a^{\frac{1}{2}}A$, $h \mapsto h' = ha^{-\frac{1}{2}}z^{-1}$; then the magnetic energy becomes $\kappa^{-1}h^{-2}z\int \omega(x)^2|\partial' A'|^2\,dx'$ where factors a^{-1} and az come from substitution $A = a^{-\frac{1}{2}}A'$ and scaling respectively. We need to multiply it by a (as we multiplied an operator); plugging $h^{-2} = h'^{-2}a^{-1}z^{-2}$ we get the same expression as before but with $z' = 1$, $a' = 1$ and $h' = ha^{-\frac{1}{2}}z^{-1} \le 1$ and $\kappa' = \kappa z$ instead of h and κ. If we establish here an error $O(h'^{-\frac{4}{3}})$ the final error will be $O(a^{-1}h'^{-\frac{4}{3}}) = O(a^{-\frac{1}{3}}h^{-\frac{4}{3}}z^{\frac{4}{3}})$.

(ii) On the other hand, let $z \le a^{-\frac{1}{2}}h$. Recall, we assume that $a \ge C_0h^2$. Then we can apply the same arguments as before but with $\bar{z} = a^{-\frac{1}{2}}h$ and we arrive to the same situation as before albeit with $h' = 1$, $a' = 1$, $\kappa' = \kappa a^{-\frac{1}{2}}h$ and with $z' = z/\bar{z}$. Then we have the trivial error estimate $O(a^{-1}) = O(a^{-\frac{1}{3}}h^{-\frac{4}{3}})$.

[4] As z denotes z_j we assume only that $z_1 + ... + z_M \asymp 1$.

5.2 Main results

Combining results of the previous subsections with proposition 2.7 we arrive to

Theorem 5.2. *If* $M \ge 2$, $\kappa \le \kappa^*$ *and* (2.30) *holds with* $\nu > \frac{4}{3}$ *then*

$$\mathsf{E}^* = \int \mathsf{Weyl}_1(x)\,dx + 2\sum_j z_j^2 S(z_j\kappa)h^{-2} + O(R_1 + R_2) \tag{5.12}$$

with

$$R_1 = \begin{cases} h^{-\frac{4}{3}} & a \ge 1 \\ a^{-\frac{1}{3}}h^{-\frac{4}{3}} & h^2 \le a \le 1 \end{cases} \tag{5.13}$$

and

$$R_2 = \kappa h^{-2} \begin{cases} a^{-3} & a \ge |\log h|^{\frac{1}{3}}, \\ |\log h^2/a|^{-1} & h^2 \le a \le |\log h|^{\frac{1}{3}} \end{cases}. \tag{5.14}$$

Proof. To prove theorem we need to prove an estimate

$$\frac{1}{\kappa h^2}\|\partial A\|^2_{\{b \le \ell(x) \le 2b\}} \le CR_2 \tag{5.15}$$

where $R_* \le b \le a$ is a "cut-off". On the other hand we know that

$$\frac{1}{\kappa^2 h^2}\|\partial A\|^2 = -\frac{\partial S}{\partial \kappa} = O(1) \tag{5.16}$$

and we need to recover the last factor in the definition of R_2.

As $a \ge 1$ we can have a^{-3} because in virtue of (2.31) the square of the partial norm in (5.16) does not exceed $Ca^{-3}\kappa^2$.

On the other hand, as $h^2 \le R_* \le a$ we can select $b : R_* \le b \le a$ such that he partial norm in (5.16) does not exceed $C|\log(a/h^2)|^{-1} \cdot \|\partial A\|^2$. $\square$

Remark 5.3. (i) As $a \le |\log h|$ we do not need assumption (2.30);

(ii) In particular, as $a \ge 1$ and $\kappa \le a^3 h^{\frac{2}{3}}$ remainder estimate is $O(h^{-\frac{4}{3}})$.

5.3 Problems and remarks

Problem 5.4. *(i) As $\kappa \in [0, \kappa^*]$ with small enough κ^* does $S(\kappa)$ really depend on κ or $S(\kappa) = S(0)$?*

(ii) If $S(\kappa)$ really depends on κ, what is asymptotic behavior of $S(\kappa) - S(0)$ as $\kappa \to +0$: can one improve $S(\kappa) - S(0) = O(\kappa)$?

Any estimate better than $O(\kappa)$ would improve (with respect to κ) remainder estimates in theorems 4.3 and 5.2.

Problem 5.5. *Improve (as $a \geq 1$) estimates in theorem 4.3 and 5.2 to those achieved in section 12.5 of [I4] for $\kappa = 0$ (i.e. without self-generated magnetic field). Namely there we were able to achieve $O(h^{-1})$ or even better, up to $O(h^{-1+\delta})$ [5].*

(i) The best outcome would be the same estimate $O(h^{-1})$ (or better [5]) for all $\kappa \in [0, \kappa^*]$.

(ii) Alternatively, we would like to see estimate $O(h^{-1} + \kappa^{\mu} h^{-\frac{4}{3}})$; in particular we would get estimate $O(1)$ for $\kappa = O(h^{2/(3\mu)})$ with exponent μ as large as possible.

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